Progress in the Development of High Energy Dense Oxidizers based on CHNO(F)-compounds

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Abstract:

Here we report about the synthesis of several new compounds with positive oxygen balances Ω as potential high energy dense oxidizers. We focused on nitramines and nitrocarbamates in combination with the trinitromethyl and fluorodinitromethyl moiety. The prepared materials were characterized thoroughly using vibrational spectroscopy (IR and Raman), multinuclear NMR spectroscopy, mass spectrometry, elemental analysis as well as DSC measurements and single crystal X-ray diffraction. In addition, the performances regarding the specific impulse I_{sp} were estimated by calculation using the EXPLO5 computer code, with heats of formation calculated at the CBS-4M level of theory and densities obtained from X-ray measurements. The sensitivities towards impact and friction were determined according BAM standard methods, as well as a small scale electrical discharge device (OZM).

Keywords: high energy dense oxidizer; polynitro compounds; sensitivities; specific impulse; single crystal X-ray diffraction

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